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Published in:
Solid State Communications

DOI:
[10.1016/S0038-1098\(01\)00057-6](https://doi.org/10.1016/S0038-1098(01)00057-6)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2001

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Palasantzas, G., & de Hosson, J. T. M. (2001). The effect of mound roughness on the electrical capacitance of a thin insulating film. *Solid State Communications*, 118(4), 203 - 206.
[https://doi.org/10.1016/S0038-1098\(01\)00057-6](https://doi.org/10.1016/S0038-1098(01)00057-6)

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Solid State Communications 118 (2001) 203–206

**solid
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communications**

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The effect of mound roughness on the electrical capacitance of a thin insulating film

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Received 4 December 2000; accepted 25 January 2001 by P. Burlet

Abstract

We investigate the influence of the roughness at a nanometre scale on the electrical capacitance of thin films. It is shown that the surface roughness causes an increase of the electrical capacitance depending on the details of the roughness characteristics. For mound rough surfaces, the increase of the electrical capacitance depends strongly on the relative magnitude of the average mound separation λ and the system correlation length ζ . A rather complex behaviour develops for $\zeta > \lambda$, whereas for $\zeta < \lambda$ a smooth decrease of the capacitance as a function of the average mound separation λ occurs due to surface smoothing. Depending on the film thickness, the presence of roughness strongly influences the electrical capacitance as long as $\zeta < \lambda$, whereas a precise determination of the actual effect requires a detailed knowledge of the thickness dependence of the roughness parameters during film growth. © 2001 Elsevier Science Ltd. All rights reserved.

PACS: 77.55.+f; 73.61.-r; 73.90.+f; 77.90.+k

Keywords: A. Thin films; A. Surfaces and interfaces; A. Insulators

Deviations of surfaces and interfaces from flatness as well as the presence of defects (e.g. dislocations, impurities, etc.) may alter the operation of microelectronic devices [1,2]. Therefore, considerable research is devoted to understand the electrical properties of devices affected by these imperfections, which might otherwise prevent device applications such as storage capacitors for dynamic and static random access memories, alternating current thin film electroluminescent devices, etc. [3–6]. Although many proposed new geometries require the growth of high quality films, kinetic effects may induce random roughness formation depending on the growth conditions.

In particular, it has been shown that random rough surfaces influence the image potential of a charge situated in the vicinity of a dielectric interface, leading by shifting electronic energy levels to an inversion layer at a semiconductor/oxide interface [7–10]. In addition, interface roughness has been shown to affect the electrical conductivity of semiconducting and metallic thin films [11–19].

Further, the presence of a rough metal/insulator interface (e.g. for polycrystalline and multi-layer BaTiO_3 thin films) influences the field breakdown mechanism [5]. Finally, a self-affine fractal roughness characterized by a roughness exponent H , a rms roughness amplitude w , and a correlation length ξ , causes a significant increase in the electric field, capacitance and leakage current in thin film capacitors [20].

For a parallel thin film plate capacitor, e.g. fabricated by the deposition of a dielectric film such as Ta_2O_5 , Al_2O_3 , SiO_2 between two metal electrodes [5,11–19,21–23], the capacitance C depends on dielectric film thickness h_0 as $C \sim 1/h_0$. A change of h_0 allows any capacitance value to be obtained which is limited, however, by defects such as pinholes in the dielectric film [21–23] and the roughness at the metal/dielectric interface [3–4,20]. Although an investigation was performed earlier for the case of a self-affine roughness on thin film capacitors, the growth front can be rough in the sense that multi-layer step structures are formed in the form of mounds [24–28]. So far, a theoretical investigation of a mound surface roughness remained unexplored, and will be the topic of the present article.

We consider a parallel-plate capacitor with only one rough electrode surface and the other is smooth. In order

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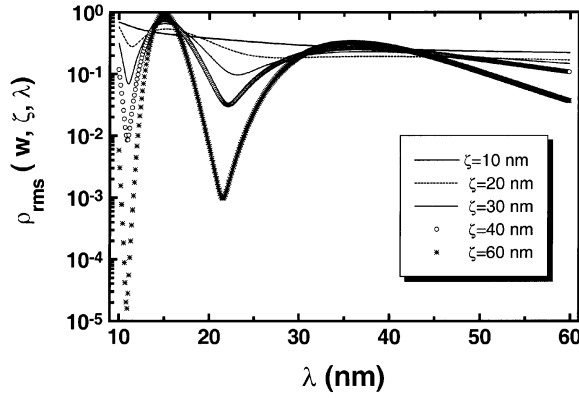


Fig. 1. Rms local surface slope $\rho_{\text{rms}} = \langle |\nabla h|^2 \rangle^{1/2}$ as a function of the average mound separation λ for various correlation lengths ζ , $w = 1$ nm and $a_0 = 0.3$ nm.

to calculate the electrical capacitance, one needs to solve the Laplace equation for the electrostatic potential Φ between the capacitor planes $\nabla^2 \Phi(x, y, z) = 0$ obeying the boundary conditions $\Phi(x, y, z = 0) = 0$ and $\Phi(x, y, z = f(x, y)) = V$ with $z = h_0 + h(\vec{p})$ (with h 's the roughness fluctuations and $\vec{p} = (x, y)$ the in-plane position vector) the rough electrode surface held at potential V [20]. Perturbation theory up to second order yields the electric field $E = -\nabla \Phi$ in a series expansion [20], which further allows the calculation of the capacitance. The surface charge density σ on the rough capacitor plate is given by $\sigma = \epsilon E \cdot \hat{n}$ with $\hat{n} = (-\hat{e}_3 \nabla h) / [1 + (\nabla h)^2]^{1/2}$ being the unit vector normal to the rough surface plate at $z = h_0 + h(\vec{p})$. Upon ensemble averaging over possible roughness configurations and assuming statistically stationary surfaces up to the second

order it follows that $\langle \tilde{h}(k) \tilde{h}(k') \rangle = [(2\pi)^4 / A] \langle |\tilde{h}(k)|^2 \rangle \delta(k + k')$. Assuming a weak surface roughness, i.e. $|\nabla h| < 1$, the average electric capacitance $C = \langle Q \rangle / V = \int \langle \sigma \rangle ds / V$ is given by Ref. [20]

$$C = C_0 \left\{ 1 + \frac{(2\pi)^5}{A} \left[2 \int_{0 < k < k_c} k^2 \langle |h(k)|^2 \rangle dk + \frac{2\pi}{h_0} \int_{0 < k < k_c} \frac{\cosh(kh_0)}{\sinh(kh_0)} k \langle |h(k)|^2 \rangle dk \right] \right\} \quad (1)$$

with ϵ being the dielectric constant of the filling material in a capacitor. A represents the average flat surface area and $C_0 = A\epsilon/h_0$, the capacitance for flat electrode surfaces.

To calculate the effect of morphology on the capacitance C by means of Eq. (1), the knowledge of the roughness spectrum $\langle |h(k)|^2 \rangle$ is required for mound roughness. In the past mound rough surfaces have been described by the interface width w , the system correlation length ζ determining how randomly the mounds are distributed on the surface, and the average mound separation λ [28]. During growth the mounds coarsen with the mound separation λ . Such a rough morphology can be described by the height–height correlation function $C(r) = \langle h(r)h(0) \rangle = w^2 e^{-(r/\zeta)^2} J_0(2\pi r/\lambda)$, where its Fourier transform $\langle |h(k)|^2 \rangle$ reads of the form [28]

$$\langle |h(k)|^2 \rangle = \frac{A}{(2\pi)^5} \frac{w^2 \zeta^2}{2} e^{-(4\pi^2 + k^2 \lambda^2)(\zeta^2/4\lambda^2)} I_0(\pi k \zeta^2/\lambda) \quad (2)$$

with $J_0(x)$ and $I_0(x)$ the Bessel and modified Bessel function of first kind and zero order, respectively. If $\zeta \geq \lambda$ the surface is characteristic to that caused by Schwoebel barrier effects [28]. Note that the correlation function $C(r)$ for mound roughness has an oscillatory behaviour for $\zeta \geq \lambda$ (strong

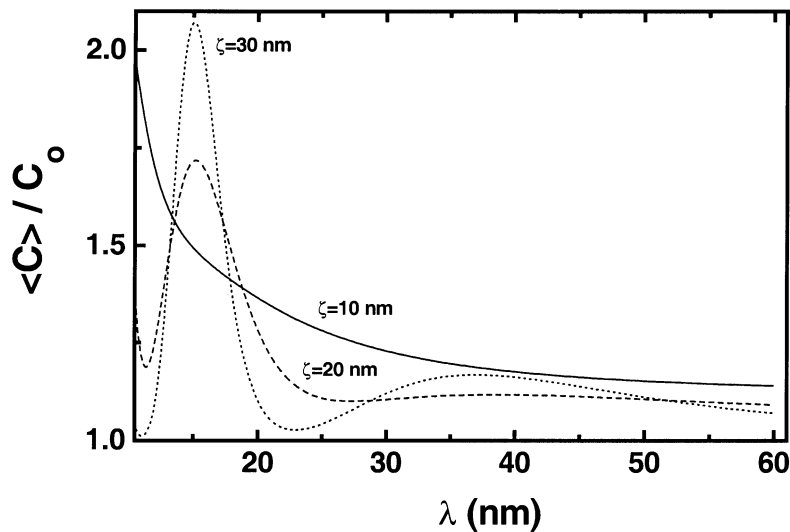


Fig. 2. Thermal capacitance ratio $\langle C \rangle / C_0$ as a function of the average mound separation λ for various correlation lengths ζ , $w = 1$ nm, $h_0 = 30$ nm, and $a_0 = 0.3$ nm.

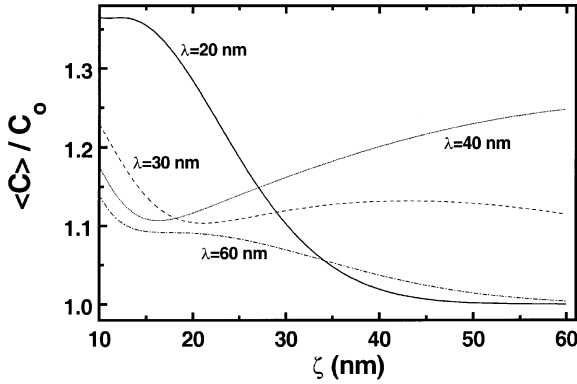


Fig. 3. Thermal capacitance ratio $\langle C \rangle / C_0$ as a function of the system correlation length ζ for various average mound separations λ , $w = 1$ nm, $h_0 = 30$ nm, and $a_0 = 0.3$ nm.

Schoweel barrier effect) leading to a characteristic satellite ring at $k = 2\pi/\lambda$ of the power spectrum $\langle |h(k)|^2 \rangle$.

The capacitance calculations were performed in the limit of weak roughness ($|\nabla h| < 1$) or alternatively small rms local surface slopes $\rho_{\text{rms}} = \langle |\nabla h|^2 \rangle^{1/2} < 1$, and small rms roughness amplitudes w such that $w \ll h_0$. Our calculations were performed in the limit of weak roughness ($|\nabla h| < 1$) or alternatively small rms local surface slopes $\rho_{\text{rms}} = \langle |\nabla h|^2 \rangle^{1/2} < 1$, and small rms roughness amplitudes $w (\ll h_0)$. Fig. 1 shows the dependence of the local surface slope as a function of the average mound separation λ for various system correlation lengths ζ . The local surface slope is given by $\rho_{\text{rms}} = \{[(2\pi)^4/A] \int_0 < k < k_c k^2 \langle |h(k)|^2 \rangle d^2 k\}^{1/2}$ which is in essence proportional to the second term in Eq. (2). Clearly for large correlation lengths $\zeta (> \lambda)$, the local slope decays in an oscillatory manner as λ increases (or the long wavelength ratio w/λ decreases leading to surface

smoothing), while for small $\zeta (< \lambda)$ the local surface slope decays exponentially as the surface smoothens (w/λ decreases).

The excess capacitance due to surface roughness depends on the rms roughness amplitude w as $C - C_0 \sim w^2$ because in general for random roughness $\langle |h(k)|^2 \rangle \sim w^2$. Fig. 2 shows the dependence of the electrical capacitance ratio $\langle C \rangle / C_0$ as a function of the average mound separation λ . $C_0 \leq \langle C \rangle$ meaning that the presence of roughness increases the electrical capacitance. Clearly, as λ increases (or w/λ decreases) $\langle C \rangle$ approaches the electrical capacitance C_0 that is characteristic for a film with a flat surface. However, for large system correlation lengths such that $\zeta > \lambda$, significant increments of $\langle C \rangle$ develop approaching finally C_0 for large mound separations $\lambda (> \zeta)$. Such an effect is special for mound roughness, whereas for any other type of roughness, like a Gaussian or a self-affine fractal roughness, a smooth approach to the electrical capacitance for films with flat surfaces will occur. This is similar to the case of $\lambda \gg \zeta$. Such an effect reflects the oscillatory behaviour of the height–height correlation function for mound roughness that takes place for $\zeta > \lambda$. Finally, as a function of the correlation length ζ (Fig. 3), the electrical capacitance shows a smooth decrement towards its value for films with flat surfaces as long as λ is small ($< \zeta$). For intermediate values of the average mound separation a more complex behaviour develops as is displayed in Fig. 3.

Finally, we will investigate the effect of roughness on the electrical capacitance as a function of film thickness. Fig. 4 shows the dependence of $\langle C \rangle / C_0$ on thickness h_0 . $\langle C \rangle / C_0$ decreases drastically with respect to the capacitance of a flat surface C_0 at small system correlation lengths ($\zeta < \lambda$). This can be understood from Eqs. (1) and (2) due to the Gaussian dependence on the ratio ζ/λ . A more precise determination of the film thickness effect needs a rather detailed

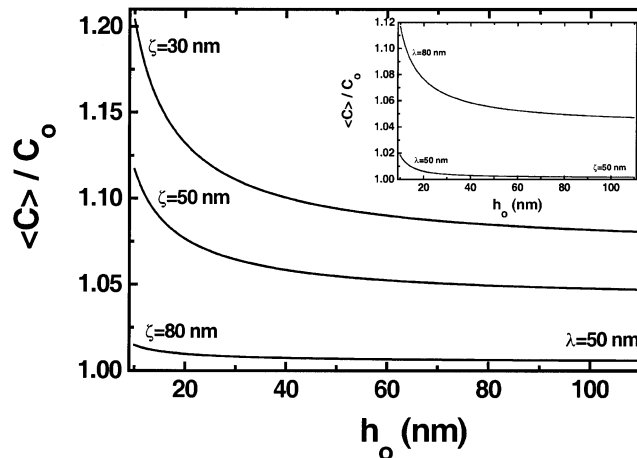


Fig. 4. Thermal capacitance ratio $\langle C \rangle / C_0$ as a function of the film thickness for various correlation lengths ζ . The inset shows a similar plot for various average mound separations λ . $w = 1$ nm, and $a_0 = 0.3$ nm for both plots.

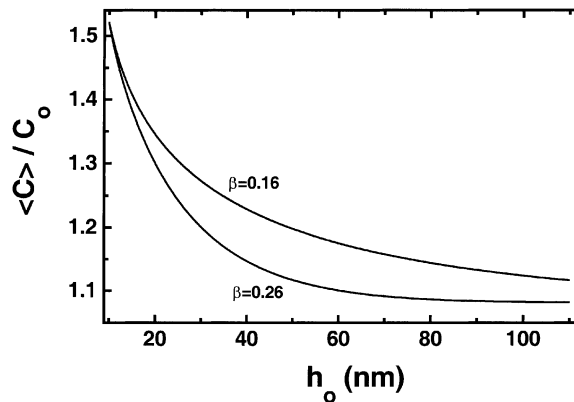


Fig. 5. Thermal capacitance ratio $\langle C \rangle / C_0$ as a function of the film thickness for film with the roughness parameters evolving with thickness as $w = 1.0(h/10)^{0.24}$ (nm), $\lambda = 10(h/10)^\beta$ (nm), and $\zeta = 20(h/10)^\beta$ (nm). The curves correspond to different growth exponents β .

knowledge of the dependence of the roughness parameters (w, ζ, λ) on film thickness. For example, it has been shown that the average mound separation and the growth time for fixed deposition rate evolve with film thickness according to $\lambda \propto h_0^\beta$ ($0.16 \leq \beta \leq 0.26$) [28]. The rms roughness amplitude varies as $w \propto h_0^{\beta'}$ ($\beta' < 1$). Therefore, in Fig. 5 we consider the thickness dependence of the ratio $\langle C \rangle / C_0$ with the roughness parameters evolving with a thickness h_0 as $w = 1.0(h/10)^{0.24}$ (nm), $\lambda = 10(h/10)^\beta$ (nm), and $\zeta = 20(h/10)^\beta$ (nm) ($\lambda > \zeta$). As Fig. 5 indicates different growth exponents β have a strong contribution on the electrical capacitance ratio $\langle C \rangle / C_0$ depending on the film thickness h_0 . It clearly illustrates the necessity of a detailed knowledge of the growth aspects.

In summary, we have investigated the effects of roughness on the electrical capacitance of thin films with one smooth boundary and the other rough at nanometre length scales. Qualitatively, similar results would be expected for films with double-rough boundaries, as well as for other geometries. We found that the roughness may cause a strong increase of the electrical capacitance. For mound rough surfaces, such an increase depends on the relative magnitude of the average mound separation λ , and on the correlation length ζ . A rather complex behaviour develops for $\zeta > \lambda$, whereas a smooth decrease of the electrical capacitance as a function of λ occurs for $\zeta < \lambda$. The presence of roughness significantly affects the electrical capacitance (depending on film thickness) as long as $\zeta < \lambda$. A precise determination of the actual effect requires a detailed knowledge of the thickness dependence of the corresponding roughness parameters during film growth.

Acknowledgements

We would like to acknowledge financial support from the 'Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO),' as well as useful discussions with Y.-P. Zhao (Rensselaer Polytechnic Institute, USA).

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